

Tioclorim [ISO]
68925-41-7 | DTXSID30218994

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 340 °C

Global applicability domain: Outside

Local applicability domain index: 2.24e-01

Confidence level: 7.80e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Desmetryn

Measured: 345

Predicted: 341

[Image not found](#)

3-Methyl-1-phenyl-1H-pyrazol-5-amine

Measured: 333

Predicted: 334

[Image not found](#)

Ametryn

Measured: 345

Predicted: 341

[Image not found](#)

1,2,4-Triaminobenzene

Measured: 340

Predicted: 315